Mechanistic Studies of Olefin and Alkyne Trimerization with Chromium Catalysts – Deuterium Labeling and Studies of Regiochemistry Using a Model Chromacyclopentane Complex

Theodor Agapie, Jay A. Labinger,* and John E. Bercaw*

Arnold and Mabel Beckman Laboratories of Chemical Synthesis, California Institute of Technology, Pasadena, CA 91125 (U. S. A.)

Supporting Information

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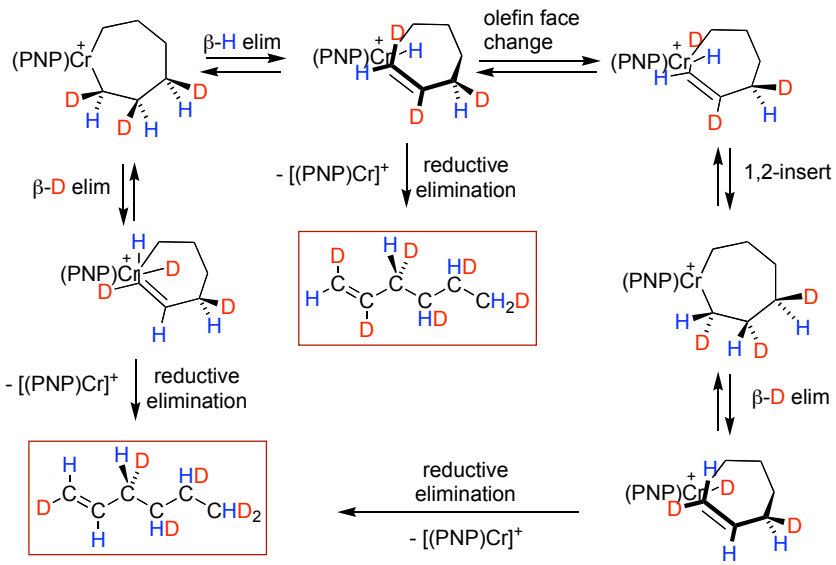

Scheme 1. Partial mechanism of the trimerization of *cis*-ethylene-d_2 showing the lack of effect of 1,2-H reinsertion on the final products.

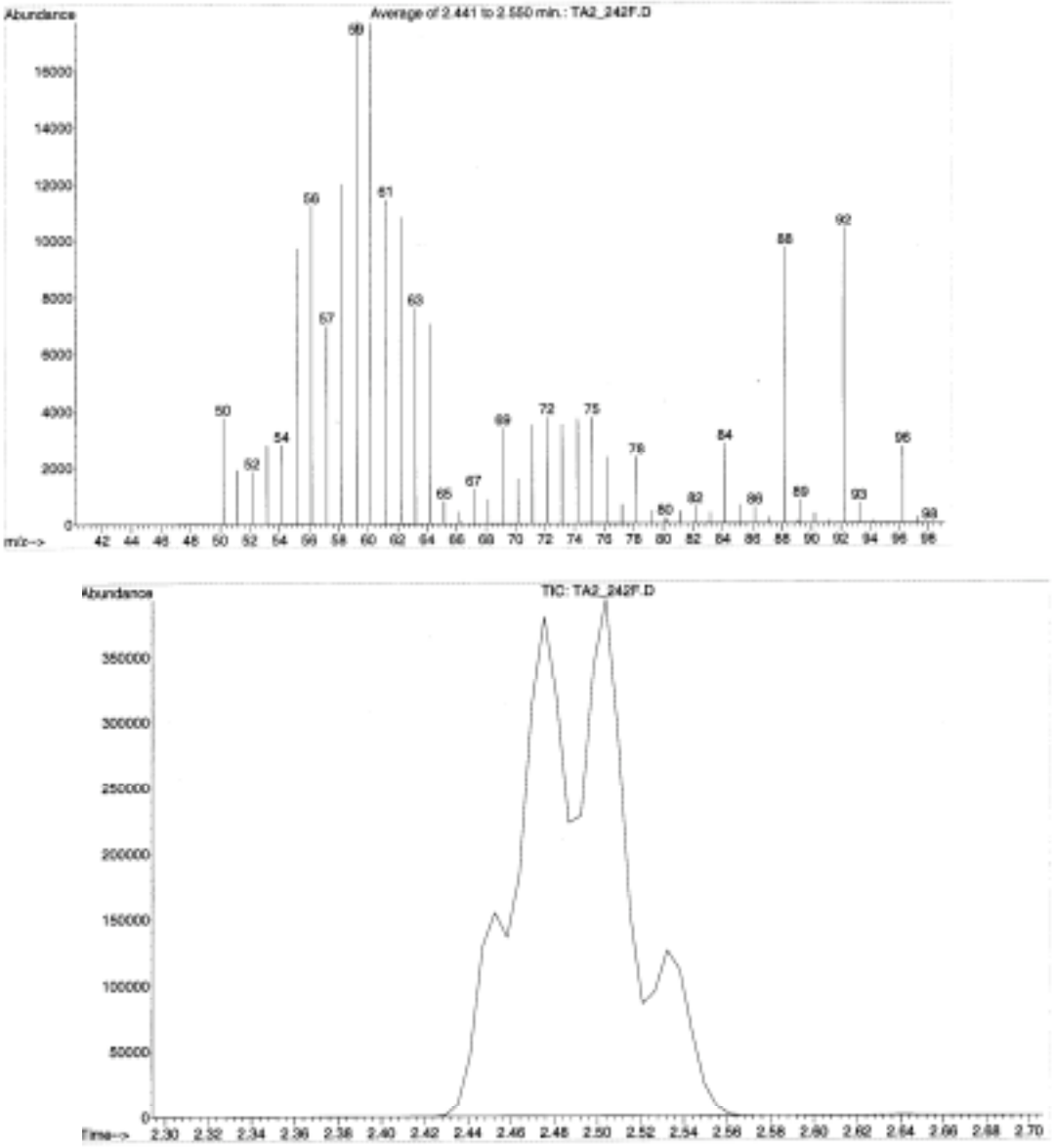

Figure 1. Typical MS (top) and GC (bottom) of the 1-hexene generated by chromium/PNP^{O4} catalysts with a C_2D_4/C_2H_4 mixture.

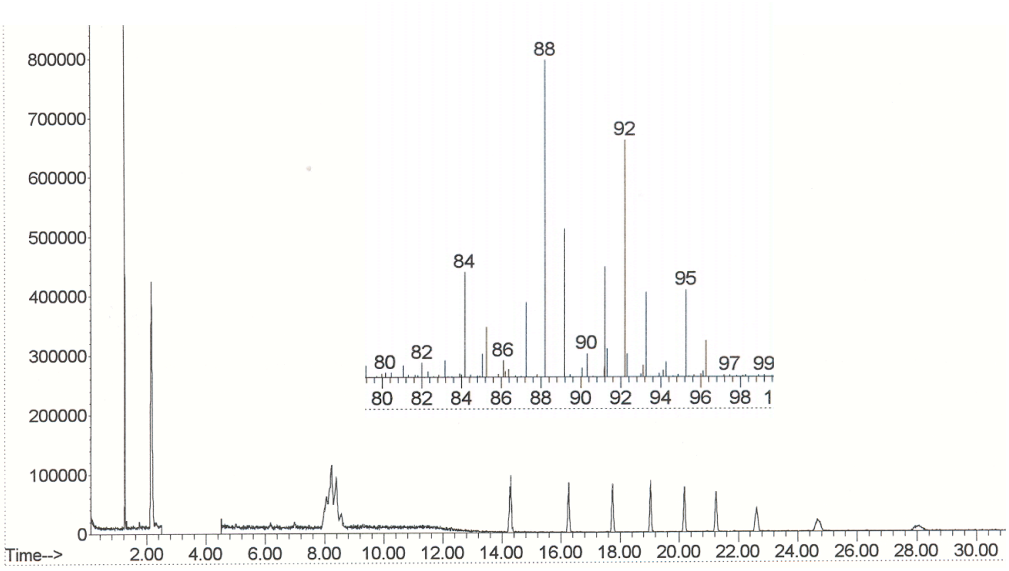

Figure 2. GC of the oligomers generated by $Ni(Ph_2PCH_2COO)(PPh_3)(Ph)$ with C_2D_4/C_2H_4 and MS (inset) of the 1-hexene fraction.

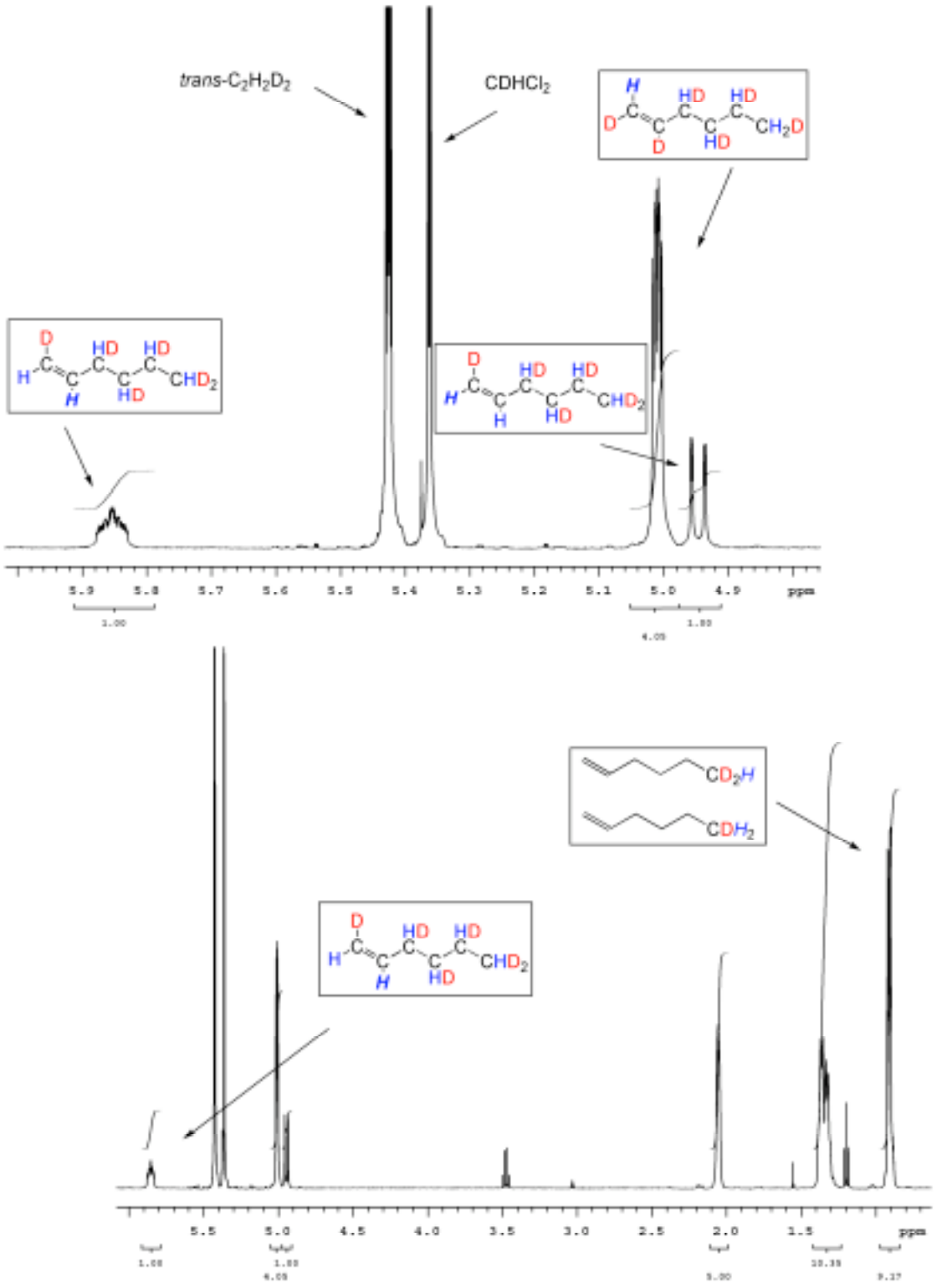

Figure 3. ^{1}H NMR spectrum of the volatile materials resulting from the trimerization of *trans*-dideuteroethylene.

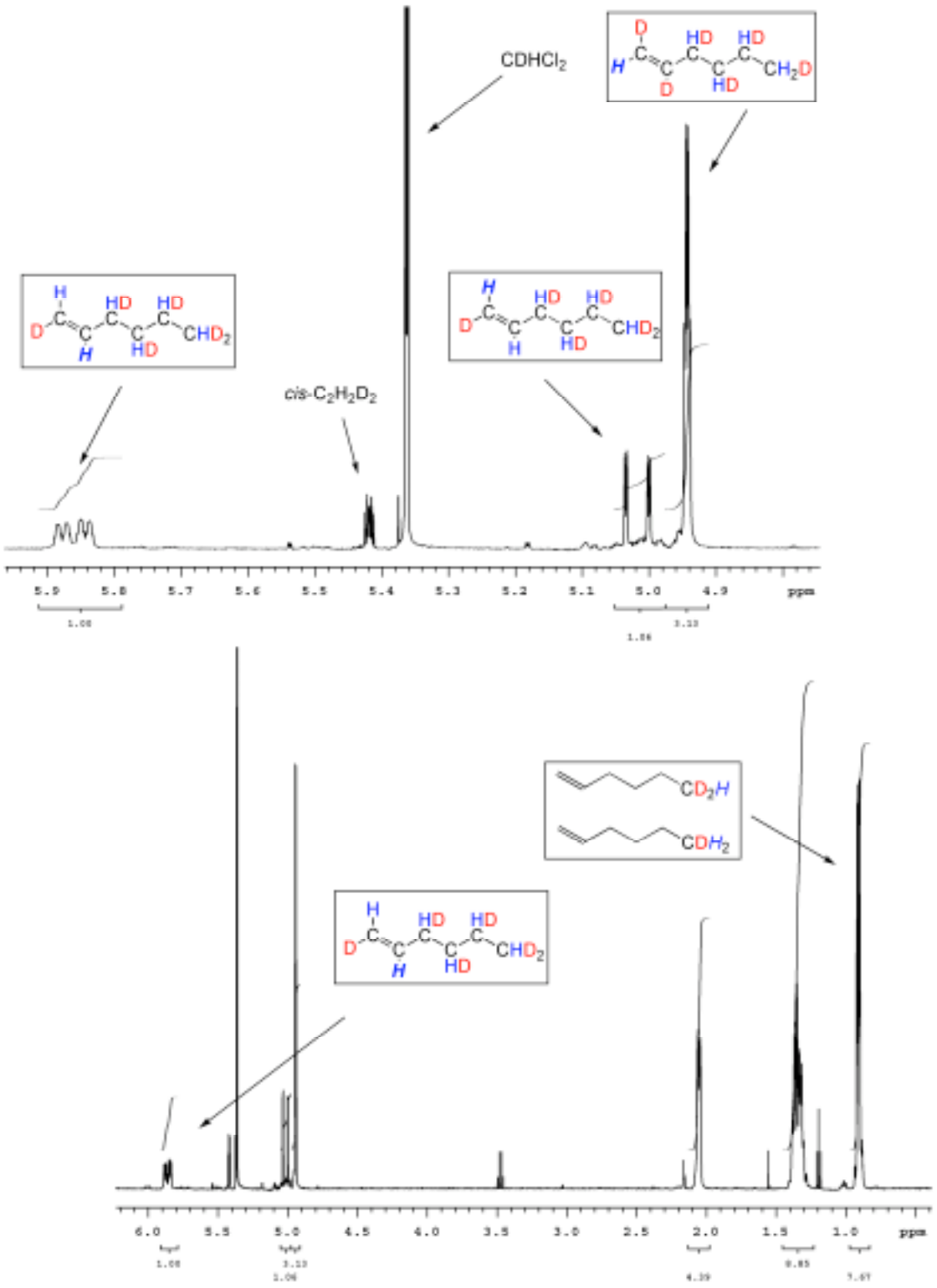

Figure 4. ^{1}H NMR spectrum of the volatile materials resulting from the trimerization of *cis*-dideuteroethylene.

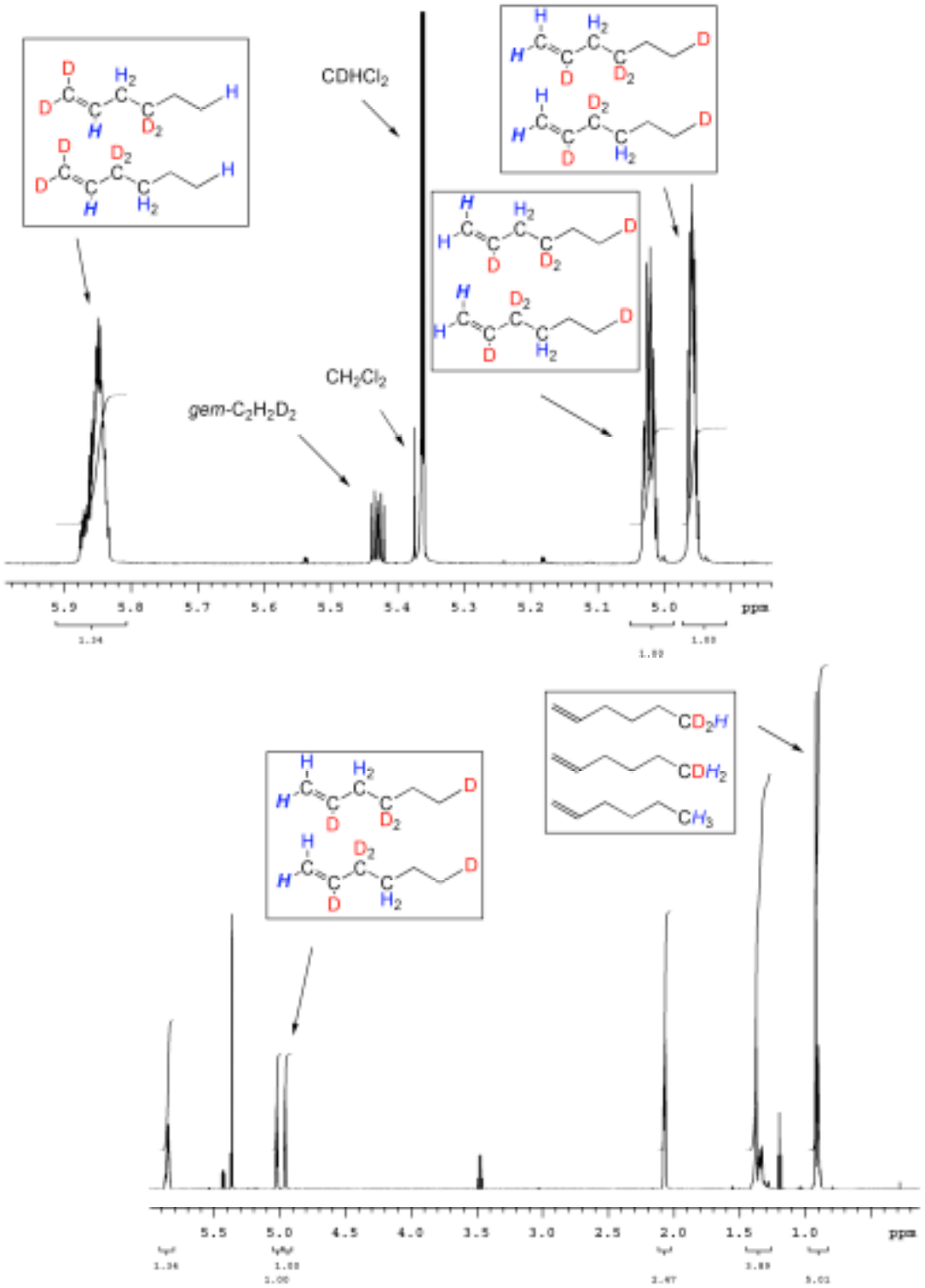

Figure 5. ^{1}H NMR spectrum of the volatile materials resulting from the trimerization of *gem*-dideuteroethylene.

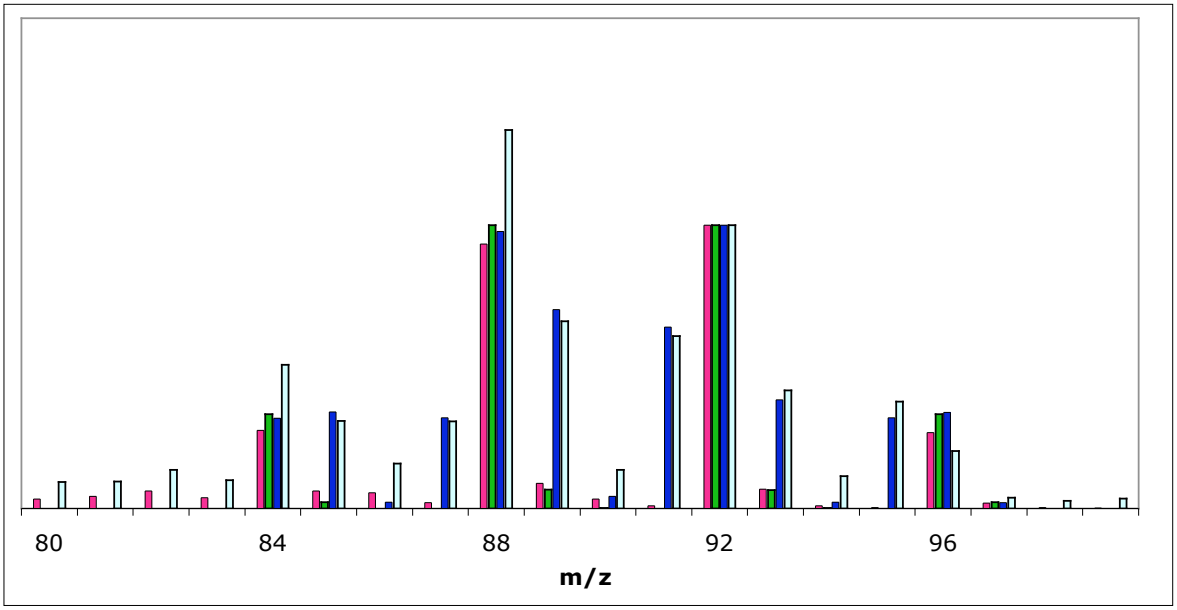

Figure 6. Red - experimental MS data for a chromium ethylene trimerization reaction. Green - simulated isotopolog distribution for a mechanism involving metallacyclic intermediates. Blue - simulated isotopolog distribution for a Cossee-type mechanism. Light blue - experimental MS data for a nickel ethylene oligomerization reaction. All intensities are normalized to same value at m/z =92.